19. (Twice Amended) A method of using a computer for evaluating the ability of a chemical entity to associate with a crystallized molecule or molecular complex comprising a calcineurin A (CnA) binding pocket defined by structure coordinates of CnA amino acids 90, 91, 92, 118, 120, 121, 122, 150, 151, 156, 160, 199, 232, 253, 254, 256, 281, 282, 283, 284, 306, 311, 312, and 317 according to Figure 1, or a homologue of said molecule or molecular complex wherein said homologue comprises a CnA homologue binding pocket that has a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5Å;

wherein said computer comprises a machine-readable data storage medium comprising a data storage material encoded with said structure coordinates defining said binding pocket and wherein said method comprises the steps of:

a. employing computational means to perform a fitting operation between the chemical entity and the CnA binding pocket or the CnA homologue binding pocket;

b. analyzing the results of said fitting operation to quantify the association between the chemical entity and the CnA binding pocket or the CnA homologue binding pocket; and

c. outputting said quantified association to a suitable output hardware.

20. (Twice Amended) A method of using a computer for evaluating the ability of a chemical entity to associate with a crystallized molecule or molecular complex

comprising a CnA binding pocket defined by structure coordinates of CnA amino acids 90, 91, 92, 118, 120, 121, 122, 150, 151, 156, 160, 199, 281, 282, 283, 306, 311, 232, and 254, according to Figure 1, or a homologue of said molecule or molecular complex, wherein said homologue comprises a CnA homologue binding pocket that has a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5 Å;

wherein said computer comprises a machine-readable data storage medium comprising a data storage material encoded with said structure coordinates defining said binding pocket and wherein said method comprises the steps of:

a. employing computational means to perform a fitting operation between the chemical entity and the CnA binding pocket or the CnA homologue binding pocket;

b. analyzing the results of said fitting operation to quantify the association between the chemical entity and the CnA binding pocket or the CnA homologue binding pocket; and

c. outputting said quantified association to a suitable output hardware.

21. (Twice Amended) A method of using a computer for evaluating the ability of a chemical entity to associate with a crystallized molecule or molecular complex comprising a CnA/CnB binding pocket defined by structure coordinates of CnA amino acids 122, 124, 159, 160, 310, 312, 313, 314, 339, 341, 343, 344, 345, 347, 351, 352, 353, 354, 355, 356, 359, 360, and 363; and calcineurin B (CnB) amino acids 49, 50, 114, 115,

118, 119, 121, 122, 123, 124, 157, 158, 159, 161, and 162 according to Figure 1, or a homologue of said molecule or molecular complex, wherein said homologue comprises a CnA/CnB homologue binding pocket that has a root mean square deviation from the backbone atoms of said CnA and CnB amino acids of not more than 1.5 Å;

wherein said computer comprises a machine-readable data storage medium comprising a data storage material encoded with said structure coordinates defining said binding pocket and wherein said method comprises the steps of:

a. employing computational means to perform a fitting operation between the chemical entity and the CnA/CnB binding pocket or the CnA/CnB homologue binding pocket;

b. analyzing the results of said fitting operation to quantify the association between the chemical entity and the CnA/CnB binding pocket or the CnA/CnB homologue binding pocket; and

c. outputting said quantified association to a suitable output hardware.

D1

Please add claims 25-30 as follows:

D2

25. (Added) A method for identifying a compound capable of associating with a molecule comprising a CnA-like binding pocket comprising the steps of:

a. using the atomic coordinates of CnA amino acids 90, 91, 92, 118, 120, 121, 122, 150, 151, 156, 160, 199, 232, 253, 254, 256, 281, 282, 283, 284, 306,

311, 312, and 317 according to Figure 1 ± a root means square deviation from the backbone atoms of said amino acids of not more than 1.5 Å, to generate a three-dimensional structure of a molecule comprising a CnA-like binding pocket;

b. employing said three-dimensional structure to design or select said compound;

c. synthesizing said compound; and

d. contacting said compound with said molecule to determine the ability of said compound to interact with said molecule.

26. (Added) A method for identifying a compound capable of associating with a molecule comprising a CnA-like binding pocket comprising the steps of:

a. using the atomic coordinates of CnA amino acids 90, 91, 92, 118, 120, 121, 122, 150, 151, 156, 160, 199, 281, 282, 283, 306, 311, 232, and 254 according to Figure 1 ± a root means square deviation from the backbone atoms of said amino acids of not more than 1.5 Å, to generate a three-dimensional structure of a molecule comprising a CnA-like binding pocket;

b. employing said three-dimensional structure to design or select said compound;

c. synthesizing said compound; and

d. contacting said compound with said molecule to determine the ability of said compound to interact with said molecule.

27. (Added) A method for identifying a compound capable of associating with a molecule comprising a CnA/CnB-like binding pocket comprising the steps of:

a. using the atomic coordinates of CnA amino acids 122, 124, 159, 160, 310, 312, 313, 314, 339, 341, 343, 344, 345, 347, 351, 352, 353, 354, 355, 356, 359, 360, and 363; and CnB amino acids 49, 50, 114, 115, 118, 119, 121, 122, 123, 124, 157, 158, 159, 161, and 162 according to Figure 1 ± a root means square deviation from the backbone atoms of said amino acids of not more than 1.5 Å, to generate a three-dimensional structure of a molecule comprising a CnA/CnB-like binding pocket;

b. employing said three-dimensional structure to design or select said compound;

c. synthesizing said compound; and

d. contacting said compound with said molecule to determine the ability of said compound to interact with said molecule.

28. (Added) The method according to claim 25 or 26, wherein in step a), the atomic coordinates of a second binding pocket defined by CnA amino acids 122, 124, 159, 160, 310, 312, 313, 314, 339, 341, 343, 344, 345, 347, 351, 352, 353, 354, 355, 356, 359, 360, and 363; and CnB amino acids 49, 50, 114, 115, 118, 119, 121, 122, 123, 124, 157, 158, 159, 161, and 162 according to Figure 1 ± a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5 Å are used.

29. (Added) The method according to claim 28, wherein in step a), the atomic coordinates of the entire set of structure coordinates of CnA and CnB according to